Predictive Science Academic Alliance Program (PSAAP)

The slides that follow were presented at the PSAAP Bidder's Meeting, May 16-17, 2006 and represent the ASC Trilab authors and interests as presented in the associated White Paper for this subject area.

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Application Domains of Interest to NNSA

A presentation to the Bidders Meeting,
NNSA Predictive Science Academic Alliance Program (PSAAP)
Dallas, Texas

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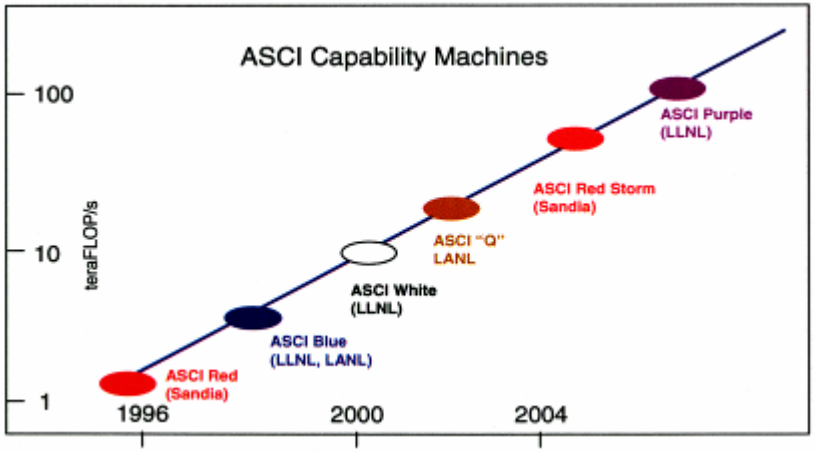
The ASCI Initiative has evolved into the ASC Program

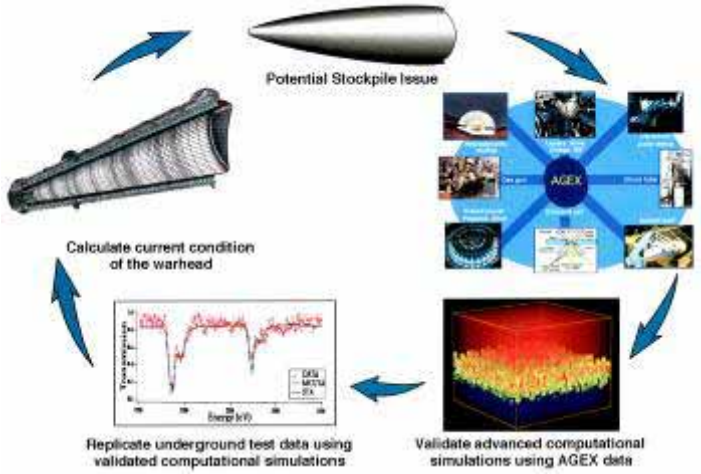
Goals for ~1996-2004
Accelerated Strategic Computing Initiative

- **Focus was on creating a new capability and demonstrating:**
  - **3D full-system simulation**
  - **functional, scalable capability platforms and infrastructure**
- **Establish simulation science and tools for Stockpile Stewardship**

Goals for Future
Advanced Simulation and Computing

- **Focus today is on employing capabilities and moving toward a predictive capability:**
  - **address national security needs**
  - **replace phenomenology in codes with science-based models**
- **Quantify and improve confidence in prediction through simulation ("Predictive Science")**



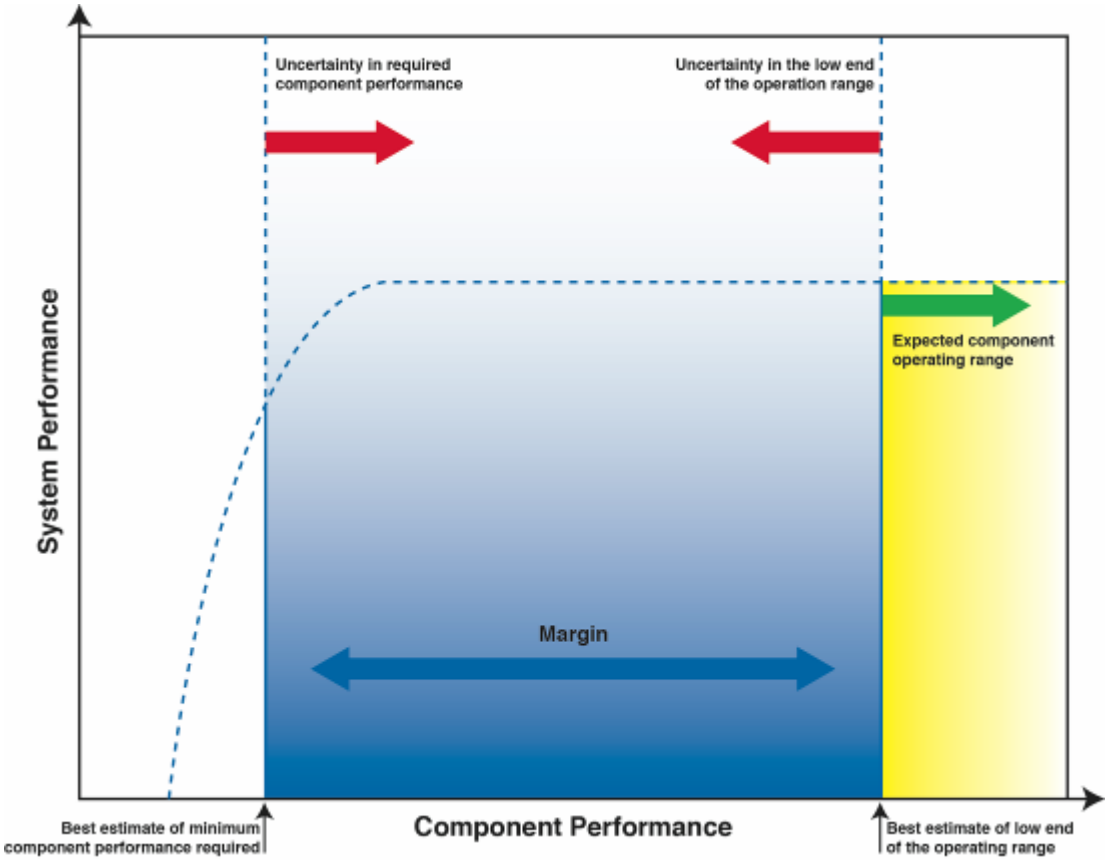


ASC simulation capabilities will be used to maintain confidence in an aging stockpile and enable transformation to a Responsive Infrastructure

The U.S. methodology for certification without testing is QMU (Quantification of Margins and Uncertainties)

QMU involves:

- **Developing a watch list of potential failure mode**
- **Establishing margins and uncertainties for these potential failure modes**



If Margin > Uncertainty, then M/U > 1, ⇒ Confidence

The new PSAAP Program has similarities and differences from the previous academic alliance program

Similarities:

- Focus on large-scale, 3D, multi-scale, multi-disciplinary integrated applications
- The universities work on unclassified, nonweapons applications

Key differences:

- Require stronger direct connection to NNSA interests for the applications and associated sub-disciplines
- Much stronger emphasis on verification, validation, and prediction methodologies and results
  - as research topics
  - demonstrated via the proposed simulations

The purpose: establish validated, large-scale, multidisciplinary, simulation-based *Predictive Science* as a major academic and applied research focus area

The PSAAP "Program Statement" identifies research areas of importance to the NNSA laboratories

- Verification and Validation and Uncertainty Quantification /Uncertainty Analysis
- Equation of State (EOS) /Constitutive Properties
- Material Damage and Failure
- Plasma Physics
- Particle Transport
- Novel Materials
- Nuclear Properties
- Turbulence Mixing/Hydrodynamics
- Material Stability
- Radiation Effects
- Chemical Transformations (includes energetic materials)
- Computer Science and Computational Mathematics

Presentations at this meeting will cover each of these areas

The PSAAP "Guidelines for Applications of Interest" identifies representative application areas of interest

- High energy density physics/stellar astrophysics in the mid to high energy density regime
- Condensed matter physics and materials science of strongly driven systems
- Design and response of engineered systems to extreme environments, such as fire, shock and radiation
- Hydrodynamics and fluid dynamics of multiple media involving mixing, turbulence and/or reaction
- Micro/nano scale material science and technology including synthesis, processing, integration, performance and reliability
- Chemical processes in organic materials, including energetic materials, polymers, and foams
- Materials compatibility and aging

This list, though not exhaustive, is indicative of NNSA interests

The PSAAP "Guidelines for Applications of Interest" gives examples of enabling sciences and technologies

1. **Predictability in science & engineering**
2. **Verification & validation strategies for large scale simulations***
3. Equations of state and constitutive properties*
4. Algorithms
5. Fluid dynamics, particularly turbulence and hydrodynamics*
6. Problem solving environments (the model integration frameworks and related software tools and methodologies)
7. Computer science*
8. Computational materials science and chemistry
9. Chemical transformations including HE*
10. Material damage and failure*
11. Material stability*
12. Novel materials*
13. Nuclear properties*
14. Engineering mechanics and design (including design margins under uncertainty)
15. Particle transport*
16. Radiation effects*
17. Computational aspects of dense plasmas
18. Plasma physics*
19. Molecular dynamics
20. Design of experiments for validation, including surrogate materials and environments
21. Statistical sciences, including data integration and model calibration

(*denotes white paper available at the PSAAP web site)

Successful proposals must address the first two areas, and many of the others

Some complex, multidisciplinary applications are identified as NOT being of interest for this program

1. Response to natural and man-made threats
2. Weather
3. Climate
4. Science of natural disasters (earthquakes, tsunami, etc.)
5. Infectious diseases
6. Protein dynamics
7. Eco-systems
8. Crowd behavior
9. Nuclear reactor design
10. Bioscience and Bioengineering
11. Economics and business systems
12. Logistics and agency resource deployment
13. Inertial confinement fusion energy systems
14. Internal combustion engines

These areas are certainly appropriate for large scale, predictive simulation, but are not of interest to NNSA for the PSAAP program

The focus on applications of interest is important to meeting the goals of the new PSAAP Program

- Establish validated, large-scale, multidisciplinary, simulation-based "Predictive Science" as a major academic and applied research program
  - demonstrate on problems of national interest
  - produce significant technical results
  - establish new prediction, verification, validation, and uncertainty quantification methodologies
- Improve the relevance of this program to Stockpile Stewardship and the NNSA laboratories
  - new capabilities and understanding for Predictive Science
  - talent pool capable of contributing to Predictive Science
- Increase the visibility of the program
  - in the academic community
  - across government and industry

PSAAP will help define and advance simulation-based Predictive Science as a sound basis for decisions of national importance